

The worm algorithm for the Ising model is rapidly mixing

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We prove rapid mixing of the Prokofiev-Svistunov (or *worm*) algorithm for the zero-field ferromagnetic Ising model, on all finite graphs and at all temperatures. As a corollary, we show how to rigorously construct simple and efficient approximation schemes for the Ising susceptibility and two-point correlation function.

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Markov-chain Monte Carlo (MCMC) simulation is one of the most versatile and widely-used tools applied in statistical physics. In order for MCMC algorithms to be useful however, it is crucial that they converge rapidly to stationarity.

A major breakthrough in the development of efficient MCMC algorithms for statistical-mechanical spin models was the invention of the Swendsen-Wang (SW) algorithm [1], which simulates the q -state Potts model [2]. Careful numerical studies (see e.g. [3–5]) suggest that the SW algorithm can be considerably more efficient than local single-spin flip algorithms. The SW algorithm utilizes a coupling [6] of the Potts and Fortuin-Kasteleyn models [7, 8] to perform *global* updates of the spins.

Recently however, it has been realized that some local algorithms have efficiencies comparable to, or even better than, the SW algorithm. Indeed, recent numerical studies [9, 10] of the single-bond algorithm for the Fortuin-Kasteleyn model, first studied by Sweeny [11], suggest that it is remarkably efficient, and exhibits the surprising property of critical speeding-up [9].

Another surprisingly efficient local algorithm is the *worm* algorithm introduced by Prokofiev and Svistunov [12]. Rather than simulating the original spin model, the Prokofiev-Svistunov (PS) algorithm simulates a space of high-temperature graphs, using a clever choice of local moves. In [13], a numerical study of the PS algorithm concluded that it is the most efficient algorithm currently known for simulating the susceptibility and correlation length of the three-dimensional Ising model. Numerical evidence presented in [14] also suggests it provides a very efficient method for studying the Ising two-point correlation function.

Despite the wealth of numerical evidence available for the SW, Sweeny and PS algorithms, relatively little is known rigorously about the rate at which they converge to stationarity, or *mix*. The SW algorithm is certainly the most well-studied of the three: rapid mixing has been established at all non-critical temperatures on the square

lattice [15], and the mixing of the mean-field (complete graph) Ising case [16] has recently received a very careful treatment. Lower bounds on the time required for mixing of the SW algorithm have also been established [17–19]. While no rigorous results appear to have been established directly for the Sweeny algorithm, interesting comparison results [20, 21] have recently been proved which relate its mixing to that of the SW algorithm. To our knowledge, no rigorous results have previously been reported for the PS algorithm.

In this Letter, we prove that the PS algorithm for the zero-field ferromagnetic Ising model is rapidly mixing, in a sense which we make precise below. The result holds on all finite connected graphs, at all temperatures. In particular, it holds precisely at the critical point on boxes in \mathbb{Z}^d . We are not aware of any other Markov chain for simulating the Ising model for which such a result is currently known.

As a corollary, we show how to rigorously construct simple and efficient approximation schemes for the Ising susceptibility and two-point correlation function. Given the general nature of the methods used, we are optimistic that analogous arguments can be successfully applied to PS algorithms for other models.

For an ergodic Markov chain with finite state space Ω , transition matrix P , and stationary distribution π , we define [23, 24] the *mixing time* to be

$$t_{\text{mix}}(\delta) := \min \left\{ t \in \mathbb{N} : \max_{s \in \Omega} \|P^t(s, \cdot) - \pi\|_{\text{TV}} \leq \delta \right\} \quad (1)$$

where $\delta \in (0, 1)$ and $\|\mu - \nu\|_{\text{TV}} := \max_{A \subseteq \Omega} |\mu(A) - \nu(A)|$ denotes the total variation distance between measures μ , ν on Ω . The mixing time is therefore the first time the distribution of the chain comes within distance δ of stationarity, having started at a worst-possible initial state.

We say that a family of Markov chains, defined on state spaces of increasing size, is *rapidly mixing* if $t_{\text{mix}}(\delta)$ is bounded above by a polynomial in $\log(|\Omega|)$. This implies that the chain need only visit a tiny fraction of the state

space to ensure mixing, so establishing rapid mixing is a very strong statement. For the Ising model, rapid mixing implies that although the number of configurations is exponential in the number of sites, only a polynomial number of them need be visited to ensure mixing.

Consider now the ferromagnetic zero-field Ising model on finite connected graph $G = (V, E)$ at inverse temperature β . For any $W \subseteq V$ and integer $1 \leq k \leq |V|$ let

$$\mathcal{C}_W := \{A \subseteq E : \partial A = W\}, \quad \mathcal{C}_k := \bigcup_{\substack{W \subseteq V \\ |W|=k}} \mathcal{C}_W, \quad (2)$$

where ∂A denotes the set of all odd vertices in the spanning subgraph (V, A) . Also consider the unnormalized measure on $\{A \subseteq E\}$ defined by $\lambda(A) = x^{|A|}$ with $x = \tanh \beta$. The standard high-temperature expansion of the Ising model [25] then gives the following graphical expression for the Ising correlation function

$$\left\langle \prod_{v \in W} \sigma_v \right\rangle = \frac{\lambda(\mathcal{C}_W)}{\lambda(\mathcal{C}_0)}. \quad (3)$$

The PS algorithm is defined on the configuration space $\mathcal{W} = \mathcal{C}_0 \cup \mathcal{C}_2$, with stationary distribution

$$\pi(A) \propto x^{|A|} \begin{cases} n, & A \in \mathcal{C}_0, \\ 2, & A \in \mathcal{C}_2. \end{cases} \quad (4)$$

The Ising susceptibility χ and two-point correlation function have natural expressions in terms of π

$$\chi = \frac{\beta}{\pi(\mathcal{C}_0)}, \quad \langle \sigma_u \sigma_v \rangle = \frac{n}{2} \frac{\pi(\mathcal{C}_{uv})}{\pi(\mathcal{C}_0)}. \quad (5)$$

A single step of the PS algorithm that we consider proceeds as in Alg. 1, with acceptance probabilities as given in (6).

Algorithm 1 (PS algorithm).

if $A \in \mathcal{C}_0$ **then**
 Choose a uniformly random vertex $u \in V$
else if $A \in \mathcal{C}_2$ **then**
 Choose a uniformly random vertex $u \in \partial A$
end if
 Choose a uniformly random neighbour v of u
 With probability $a(A, A \triangle uv)$, let $A \rightarrow A \triangle uv$
 Otherwise $A \rightarrow A$

Here \triangle denotes symmetric difference. For technical reasons, we consider the *lazy* version of the algorithm, in which the acceptance probability is chosen to be one half of the standard Metropolis prescription [23, 26]

$$a(A, A \triangle uv) = \frac{1}{2} \begin{cases} \min \left(1, \frac{d(u)}{d(v)} x^\pm \right), & A, A \triangle uv \in \mathcal{C}_2, u \in \partial A \\ \min(1, x^\pm), & \text{otherwise.} \end{cases} \quad (6)$$

Here x^\pm equals x if the transition adds an edge, and $1/x$ if it removes an edge, and $d(u)$ denotes the degree of u in G . If G is regular, then $a(A, A \triangle uv)$ is simply $\min(1, x^\pm)/2$.

We now state our main result.

Theorem 1. *The mixing time of the PS algorithm on a finite connected graph $G = (V, E)$ with parameter $x \in (0, 1)$ and $n = |V| \geq 2$ satisfies*

$$t_{\text{mix}}(\delta) \leq \frac{1}{2x} \left(\log \left(\frac{8}{x} \right) - \frac{\log \delta}{m} \right) \left(3 + \frac{1}{mx} \right) \Delta(G) n^6 m^2,$$

where $m = |E|$ and $\Delta(G)$ is the maximum degree.

We note that general arguments imply that implicit in Theorem 1 are bounds for other related properties of the PS algorithm, including $O(\Delta(G)n^6m)$ bounds for the relaxation time (inverse spectral gap) [23], exponential autocorrelation time [26], and all integrated autocorrelation times [26]. In the specific case of boxes in regular lattices, each of these latter quantities are then $O(n^7)$, while $t_{\text{mix}}(\delta) = O(n^8)$.

We now outline a proof of Theorem 1. A detailed proof will appear elsewhere [27]. Our argument uses the method of multicommodity flows [28, 29]. We therefore consider the *transition graph* \mathcal{G} of the PS algorithm, whose vertex set is \mathcal{W} , and whose edge set \mathcal{E} consists of those pairs of states $(A, A') \in \mathcal{W}^2$ for which the one-step transition $A \rightarrow A'$ occurs with strictly positive probability. In its simplest form, the method involves prescribing paths in \mathcal{G} between each pair of states $A, A' \in \mathcal{W}$, and showing that for the given choice of paths there are no edges in \mathcal{G} which become overly congested.

We now make these ideas precise. In the current setting, it is in fact convenient to define paths only from states in \mathcal{C}_2 to states in \mathcal{C}_0 , rather than between all pairs in \mathcal{W} . Therefore, for each pair $(I, F) \in \mathcal{C}_2 \times \mathcal{C}_0$, we fix a simple path $\gamma_{I,F}$ in \mathcal{G} from I to F , and we let $\Gamma = \{\gamma_{I,F} : (I, F) \in \mathcal{C}_2 \times \mathcal{C}_0\}$ denote the set of all such paths. Adapting Lemma 4.4 from [22] to our setting implies that for any choice of Γ we have

$$\begin{aligned} t_{\text{mix}}(\delta) &\leq \log \left(\frac{1}{\pi_{\min} \delta} \right) \left[2 + 4 \left(\frac{\pi(\mathcal{C}_2)}{\pi(\mathcal{C}_0)} + \frac{\pi(\mathcal{C}_0)}{\pi(\mathcal{C}_2)} \right) \right] \varphi(\Gamma) \\ &\leq \left(\log \left(\frac{8}{x} \right) - \frac{\log \delta}{m} \right) \left(6 + \frac{2}{mx} \right) m n \varphi(\Gamma) \end{aligned} \quad (7)$$

where $\pi_{\min} = \min_{A \in \mathcal{W}} \pi(A)$, and where the *congestion* of Γ is defined to be

$$\varphi(\Gamma) := \mathcal{L}(\Gamma) \max_{AA' \in \mathcal{E}} \left\{ \sum_{(I,F) \in \mathcal{P}(AA')} \frac{\pi(I)\pi(F)}{\pi(A)P(A, A')} \right\}.$$

Here $\mathcal{P}(e) = \{(I, F) \in \mathcal{C}_2 \times \mathcal{C}_0 : \gamma_{I,F} \ni e\}$ is the set of all pairs of states whose specified path uses the edge $e \in \mathcal{E}$,

$\mathcal{L}(\Gamma) = \max |\gamma_{I,F}|$ is the length of a longest path in Γ , and P denotes the transition matrix of the PS algorithm, as defined by Alg. 1 and (6). In obtaining the second inequality in (7) we have utilized the easily established bound [27]

$$\frac{2}{n} \frac{mx}{mx+1} \leq \frac{\pi(\mathcal{C}_2)}{\pi(\mathcal{C}_0)} \leq n-1.$$

The problem of bounding the mixing time has now been reduced to the problem of constructing an appropriate set of paths Γ for which tight bounds on the congestion $\varphi(\Gamma)$ can be obtained. We now exhibit such a set of paths. For concreteness, it is convenient to fix some arbitrary vertex labeling of G , and to use this labeling to lexicographically induce an ordering on the set of all subgraphs of G . For each cycle in G , we also use the vertex labeling to specify an arbitrary fixed orientation.

We begin by noting that in order to transition from I to F , it suffices to flip each edge in $I\Delta F$ precisely once. If $(I, F) \in \mathcal{C}_2 \times \mathcal{C}_0$, then $\partial(I\Delta F) = \partial I = \{u_I, v_I\}$ for some $u_I, v_I \in V$. By the handshaking lemma, u_I, v_I belong to the same component in $(V, I\Delta F)$. Let A_0 denote the shortest path between u_I and v_I in $(V, I\Delta F)$; if multiple shortest paths exist, use the vertex labeling to ensure A_0 is uniquely defined. Now observe that $I\Delta F \setminus A_0 \in \mathcal{C}_0$. Since every element of the cycle space \mathcal{C}_0 can be decomposed [30] into an edge disjoint union of cycles in G , we can again use the vertex labeling to obtain a unique decomposition $I\Delta F = \cup_{i=0}^k A_i$ for some k , where A_1, A_2, \dots, A_k is an ordered list of disjoint cycles.

We can now define the path $\gamma_{I,F}$ as follows. Starting in state I , we first traverse the path A_0 , starting from the lowest labeled of the two odd vertices $\{u_I, v_I\}$, and inverting the occupation status of each edge as we proceed; add the edge if it was absent, delete it if it was present. Having arrived at the intermediate state $I\Delta A_0$, we then process A_1 , then A_2, \dots . For each cycle A_i , we begin at the lowest labeled vertex, and proceed according to the fixed orientation induced by the vertex labeling. Once A_k has been processed, we have arrived in state $I\Delta(\cup_{i=0}^k A_i) = F$. We emphasize that each step in the path $\gamma_{I,F}$ corresponds to a valid step of the PS algorithm, which occurs with strictly positive probability. Let $\Gamma = \{\gamma_{I,F} : (I, F) \in \mathcal{C}_2 \times \mathcal{C}_0\}$ denote the collection of all such paths. Fig. 1 illustrates a simple example.

We now proceed to bound $\varphi(\Gamma)$ for this choice of Γ . Our argument is similar to that given in the discussion of perfect and near-perfect matchings presented in [22]. For each transition $e = AA' \in \mathcal{E}$, we introduce a map $\eta_e : \mathcal{C}_2 \times \mathcal{C}_0 \rightarrow \mathcal{W} \cup \mathcal{C}_4$ defined by $\eta_e(I, F) := I\Delta F\Delta A$. It is straightforward to show [27] that η_e is injective. We also introduce the unnormalized measure Λ on $\mathcal{W} \cup \mathcal{C}_4$

defined by

$$\Lambda(A) = x^{|A|} \begin{cases} n, & \text{if } A \in \mathcal{C}_0, \\ 2, & \text{if } A \in \mathcal{C}_2, \\ 1, & \text{if } A \in \mathcal{C}_4. \end{cases}$$

Note that for $A \in \mathcal{W}$ we have $\pi(A) = \Lambda(A)/\Lambda(\mathcal{W})$. It is again straightforward to show [27] that

$$\frac{\Lambda(I)\Lambda(F)}{\Lambda(A)} \leq n \Lambda(\eta_e(I, F)). \quad (8)$$

If $e = AA'$ is a maximally congested transition, then

$$\begin{aligned} \varphi(\Gamma) &\leq \frac{m}{P(A, A')\Lambda(\mathcal{W})} \sum_{(I, F) \in \mathcal{P}(e)} \Lambda(\eta_e(I, F)) \\ &\leq \frac{mn}{P(A, A')} \frac{\Lambda(\mathcal{W} \cup \mathcal{C}_4)}{\Lambda(\mathcal{W})} \\ &\leq mn \frac{2n\Delta(G)}{x} \frac{n^3}{8} = \frac{1}{4x} \Delta(G) n^5 m. \end{aligned}$$

The first inequality follows from (8) and the fact that $\mathcal{L}(\Gamma) \leq m$. The second follows because η_e is an injection. The third inequality then follows by noting that (3) implies $\lambda(\mathcal{C}_W) \leq \lambda(\mathcal{C}_0)$ for any $W \subseteq V$, and also noting that (6) implies $P(A, A') \geq x/(2n\Delta(G))$ for any $A \neq A'$ with $P(A, A') > 0$. This establishes Theorem 1.

As immediate corollaries of Theorem 1, we can construct fully-polynomial randomised approximation schemes (fpras) [31] for the Ising susceptibility and two-point correlation function. Both of these problems can be shown [27] to be #P-hard, by reduction to the #MAXCUT problem, which is known to be #P-complete [32]. This strongly suggests that a general solution stronger than an fpras is unlikely to exist for these problems.

Consider the susceptibility. An fpras for χ is a randomized algorithm such that for any G and β , and any $\epsilon, \eta \in (0, 1/4)$, the algorithm runs in time bounded by a polynomial in $n, \epsilon^{-1}, \eta^{-1}$, and the output \mathcal{Y} satisfies

$$\mathbb{P}[(1 - \epsilon)\chi \leq \mathcal{Y} \leq (1 + \epsilon)\chi] \geq 1 - \eta. \quad (9)$$

From (5), we see that in order to obtain an fpras for χ , it suffices to construct an fpras for $\pi(\mathcal{C}_0)$.

Let $\mathcal{A} \subseteq \mathcal{W}$ be any event for which $\pi(\mathcal{A}) \geq 1/S(n)$ with $S(n)$ a polynomial in n . Let $R(G, \mathcal{A})$ denote the upper bound for $t_{\text{mix}}(\delta)$ given in Theorem 1 with $\delta = \epsilon/[16S(n)]$. A slight refinement [27] of Lemma 3 in [32] then implies that the following algorithm defines an fpras for $\pi(\mathcal{A})$.

Algorithm 2 (fpras).

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for  $1 \leq j \leq 7 \lceil \log \eta^{-1} \rceil + 1$  do
  for  $1 \leq i \leq 20 \lceil S(n)\epsilon^{-2} + 1 \rceil$  do
    Run the PS algorithm for  $R(G, \mathcal{A})$  steps
    Let  $Y_{i,j}$  be 1 if the final state lies in  $\mathcal{A}$ , and 0 otherwise
  end for
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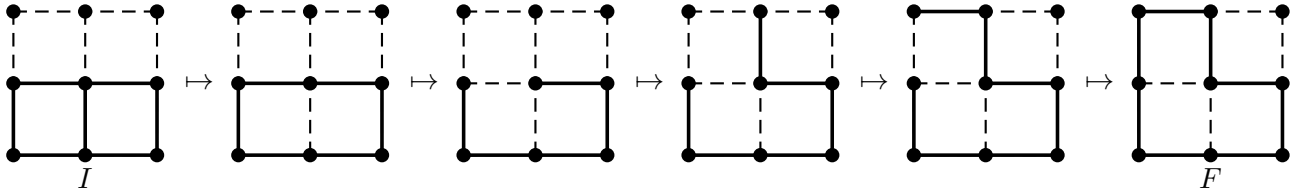


FIG. 1. Example of a path $\gamma_{I,F}$. We order the vertices from left to right, and bottom to top. $I \triangle F = A_0 \cup A_1$, where the path A_0 consists of the single edge v_2v_5 , and the cycle A_1 is $v_4v_5v_8v_7v_4$.

Compute the sample mean \bar{Y}_j of the $Y_{i,j}$
end for
 Output the median of $\{\bar{Y}_j\}$.

Since it follows [27] from (3) that $\pi(\mathcal{C}_0) \geq 1/(2n+1)$, if in Alg. 2 we let $\mathcal{A} = \mathcal{C}_0$ and choose $S(n) = (2n+1)$, we obtain an fpras for $\pi(\mathcal{C}_0)$, and hence for χ .

Similarly, fix $k \in \mathbb{N}$, and consider the problem of computing the two-point correlation function between any pair of vertices u, v of graph distance $d(u, v) \leq k$. Let $\mathcal{A} = \mathcal{C}_{uv}$, let $S(n) = n(n+1)x^{-k}/2$, and note [27] that $\pi(\mathcal{C}_{uv}) \geq 1/S(n)$. It then follows that Alg. 2 yields an fpras for $\pi(\mathcal{C}_{uv})$. Since we then have an fpras for both $\pi(\mathcal{C}_{uv})$ and $\pi(\mathcal{C}_0)$, it follows from (5) that we have an fpras for $\langle \sigma_u \sigma_v \rangle$. To prove $\pi(\mathcal{C}_{uv}) \geq 1/S(n)$, note [27] that for any fixed shortest path p_{uv} between u and v , the map $\alpha : \mathcal{C}_{u,v} \rightarrow \mathcal{C}_0$ defined by $\alpha(A) = A \triangle p_{uv}$ is a bijection, which implies $\lambda(\mathcal{C}_0) \leq x^{-d(u,v)}\lambda(\mathcal{C}_{uv})$.

We conclude with some remarks. We note that Jerrum and Sinclair [32] also considered an MCMC algorithm on a space of Ising high-temperature graphs, however their chain requires a strictly non-zero magnetic field. It can, nevertheless, be used to obtain an fpras for the Ising partition function, even in zero field.

Finally, as noted in [13], it is straightforward to establish a Li-Sokal type lower bound for the PS algorithm. In particular, this implies that near criticality on \mathbb{Z}_L^3 , the divergence of the relaxation time must be at least of order $L^{d+\alpha/\nu} \approx n^{1.06}$, while Theorem 1 implies it cannot be worse than $O(n^7)$. It would clearly be of considerable interest to further sharpen these bounds in the specific setting of \mathbb{Z}_L^3 , so as to determine the actual asymptotic behaviour of the relaxation and mixing times in that case.

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